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ORGANIC CHEMISTRY DIVISION

COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY

NOMENCLATURE OF ORGANIC CHEMISTRY. SECTION H: ISOTOPICALLY MODIFIED COMPOUNDS (First Edition)

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SECTION H: ISOTOPICALLY MODIFIED COMPOUNDS

(Approved Recommendations 1978)

INTRODUCTION

These rules provide a general system of nomenclature for organic compounds whose isotopic nuclide (ref. 1)* composition deviates from that occurring in nature. † Comparative examples of the application of these rules are given in the Appendix, p. 538.

There is one other general system in use for describing isotopically modified compounds. It is based on an extension of the principles proposed by Boughton (ref. 3) for designating compounds containing hydrogen isotopes and is currently in use mainly in the Chemical Abstracts Service index nomenclature system. For a description of its current use, see ref. 4.

The system codified in these present rules provides for recognition of various types of isotopic modification and thus was chosen over the system based on the Boughton principles.

H-1. SYMBOLS, DEFINITIONS, AND FORMULAE

Rule H-1.1. Symbols

1.11—Nuclide symbols. The symbol for denoting a nuclide in the formula or name of an isotopically modified compound consists of the atomic symbol for the element and an Arabic numeral in the left superscript position which indicates the mass number of the nuclide (ref. 5a).

1.12—Atomic symbols. The atomic symbols used in the nuclide symbol are those given in the IUPAC Inorganic Nomenclature Rules (ref. 5b). In the nuclide symbol, the atomic symbol is printed in Roman type, italicized atomic symbols being reserved for letter locants, as is customary in organic chemical nomenclature (cf. Rule C-814.4, p.255).

> Note: For the hydrogen isotopes protium, deuterium, and tritium, the nuclide symbols ^{1}H, ^{2}H, and ^{3}H, respectively, are used. The symbols D and T for ^{2}H and ^{3}H, respectively, may be used, but not when other modifying nuclides are also present because this may cause difficulties in the alphabetic ordering of the nuclide symbols in the isotopic descriptor. Although the symbols *d* and *t* have been and are still used in place of ^{2}H and ^{3}H in names formed according to the Boughton system (see Introduction), in no other cases are lower-case letters used as atomic symbols. Therefore, the use of *d* and *t* in chemical nomenclature outside of the Boughton system is not recommended.

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* References for Section H are on page 537.

† For a discussion of the meaning of 'natural composition', see ref. 2. In any context where the accuracy requires it, the natural nuclidic composition used shall be stated.

Rule H-1.2. Definitions and formulae of various types of isotopic modification

1.21—An isotopically *unmodified* compound has a macroscopic composition such that its constituent nuclides are present in the proportions occurring in nature. Its formula and name are written in the customary manner.

Examples:

1. CH_4 Methane

2. CH_3-CH_2-OH Ethanol

1.22—An isotopically *modified* compound has a macroscopic composition such that the isotopic ratio of nuclides for at least one element deviates measurably from that occurring in nature. It is either an isotopically *substituted* compound or an isotopically *labeled* compound.

1.23—An isotopically *substituted* compound has a composition such that essentially all the molecules of the compound have *only* the indicated nuclide(s) at each designated position. For all other positions, the absence of nuclide indication means that the nuclide composition is the natural one.

The formula of an isotopically *substituted* compound is written as usual except that appropriate nuclide symbols are used. When different isotopes of the same element are present at the same position, common usage is to write their symbols in order of increasing mass number.

Examples (for names see Rule H-2.11):

1. $^{14}CH_4$ (^{14}C)Methane

2. $^{12}CHCl_3$ (^{12}C)Chloroform

3. CH_3-CH^2H-OH (1-$^2H_1$)Ethanol

not

CH_3-C^2HH-OH

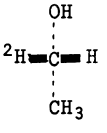
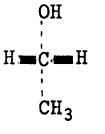
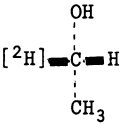
1.24—An isotopically *labeled* compound is a mixture of an isotopically unmodified compound with one or more analogous isotopically substituted compound(s).

Note: Although an isotopically labeled compound is really a mixture as far as chemical identity is concerned (in the same way as is an unmodified compound), such mixtures are called "isotopically labeled compounds" for nomenclature purposes.

1.25—An isotopically labeled compound is designated as *specifically labeled* when a *unique* isotopically substituted compound is formally added to the analogous isotopically unmodified compound. In such a case, both position(s) and number of each labeling nuclide are defined.

The structural formula of a specifically labeled compound is written in the usual way, but with the appropriate nuclide symbol(s) and multiplying subscript, if any, enclosed in *square brackets*. Other principles used in writing the formula are described in Rule H-1.23.

Examples:

	Isotopically substituted compound	when added to	Isotopically unmodified compound	gives rise to	Specifically labeled compound
1.	$^{14}CH_4$		CH_4		$[^{14}C]H_4$
2.	$CH_2{}^2H_2$		CH_4		$CH_2[^2H_2]$
3.	$CH_3-CH_2-^{18}OH$		CH_3-CH_2-OH		$CH_3-CH_2-[^{18}O]H$
4.	$CH^2H_2-CH_2-O^2H$		CH_3-CH_2-OH		$CH[^2H_2]-CH_2-O[^2H]$
5.					

Note: Although the formula for a specifically labeled compound does not represent the composition of the bulk material, which usually consists overwhelmingly of the isotopically unmodified compound, it does indicate the presence of the compound of chief interest, the isotopically substituted compound.

A specifically labeled compound is (a) *singly labeled* when the isotopically substituted compound has only one isotopically modified atom, e.g., $CH_3-CH[^2H]-OH$; (b) *multiply labeled* when the isotopically substituted compound has more than one modified atom of the same element at the same position or at different positions, e.g., $CH_3-C[^2H_2]-OH$ and $CH_2[^2H]-CH[^2H]-OH$; or (c) *mixed labeled* when the isotopically substituted compound has more than one kind of modified atom, e.g., $CH_3-CH_2-[^{18}O][^2H]$.

1.26—An isotopically labeled compound is designated as *selectively labeled* when a *mixture* of isotopically substituted compounds is formally added to the analogous isotopically unmodified compound in such a way that the position(s) but not necessarily the number of each labeling nuclide is defined. A selectively labeled compound may be considered as a mixture of specifically labeled compounds.

A selectively labeled compound may be (a) *multiply labeled* when in the unmodified compound there is more than one atom of the same element at the position where the isotopic modification occurs, e.g., H in CH_4, or there are several atoms of the same element at different positions where the isotopic modification occurs, e.g., C in C_4H_8O; or (b) *mixed labeled* when there is more than one labeling nuclide in the compound, e.g., C and O in CH_3-CH_2-OH.

Note: When there is only one atom of an element that can be modified in a compound, only specific labeling can result (see Rule H-1.25).

A selectively labeled compound cannot be described by a unique structural formula; therefore it is represented by inserting the nuclide symbols preceded by any necessary locant(s) (letters and/or numbers) but without multiplying subscripts, enclosed in square brackets directly before the usual formula or, if necessary, before parts of the formula that have an independent numbering. Identical locants are not repeated.

When different nuclides are present, the nuclide symbols are written in alphabetic order according to their symbols, or when the atomic symbols are identical, in order of increasing mass number (see Rules H-2.81 and H-2.82).

Examples:

	Mixture of isotopically substituted compounds	when added to	Isotopically unmodified compound	gives rise to	Selectively labeled compound
1.	$CH_3{}^2H$, $CH_2{}^2H_2$ CH^2H_3, C^2H_4 or any two or more of the above		CH_4		$[^2H]CH_4$
2.	$CH_3-CH_2-CH^2H-CO_2H$ $CH_3-CH_2-C^2H_2-CO_2H$		$CH_3-CH_2-CH_2-CO_2H$		$[2-^2H]CH_3-CH_2-CH_2-CO_2H$
3.	$CH_3-{}^{14}CH_2-{}^{14}CH_2-CO_2H$ $CH_3-{}^{14}CH_2-CH_2-CO_2H$ $CH_3-CH_2-{}^{14}CH_2-CO_2H$ or any two of the above		$CH_3-CH_2-CH_2-CO_2H$		$[2,3-^{14}C]CH_3-CH_2-CH_2-CO_2H$
4.	$CH_3-{}^{14}CH_2-OH$ $CH_3-CH_2-{}^{18}OH$ $CH_3-{}^{14}CH_2-{}^{18}OH$ or any two of the above		CH_3-CH_2-OH		$[1-^{14}C,{}^{18}O]CH_3-CH_2-OH$
5.	${}^{14}CH_3-CH_2-CO_2-CH_3$ $CH_3-CH_2-CO_2-{}^{14}CH_3$ ${}^{14}CH_3-CH_2-CO_2-{}^{14}CH_3$ or any two of the above		$CH_3-CH_2-CO_2-CH_3$		$[3-^{14}C]CH_3-CH_2-CO_2-[^{14}C]CH_3$

Note: The method of writing formulae as given by the above rule may also be of use if a compound is represented by its molecular formula rather than its structural formula, e.g., $[^2H]C_2H_6O$.

1.27—In a selectively labeled compound formally arising from mixing several known isotopically substituted compounds with the analogous isotopically unmodified compound, the number or the possible number of labeling nuclide(s) for each position may be indicated by subscripts to the atomic symbol(s). Two or more subscripts referring to the same nuclide symbol are separated by a semicolon. For a multiply labeled or mixed labeled compound (see Rule H-1.26), the subscripts are written successively in the same order as the various isotopically substituted compounds are considered. The subscript zero is used to indicate that one of the isotopically substituted compounds is not modified at the indicated position.

Examples:

	Mixture of isotopically substituted compounds	when added to	Isotopically unmodified compound	gives rise to	Selectively labeled compound
1.	$CH_2{}^2H\text{-}CH_2\text{-}OH$ $CH^2H_2\text{-}CH_2\text{-}OH$		$CH_3\text{-}CH_2\text{-}CH$		$[2\text{-}^2H_{1;2}]CH_3\text{-}CH_2\text{-}OH$
2.	$CH^2H_2\text{-}CH_2\text{-}OH$ $CH^2H_2\text{-}CH_2\text{-}{}^{18}OH$		$CH_3\text{-}CH_2\text{-}OH$		$[2\text{-}^2H_{2;2}, {}^{18}O_{0;1}]CH_3\text{-}CH_2\text{-}OH$ *
3.	$CH_3\text{-}CH_2\text{-}{}^{18}OH$ $CH^2H_2\text{-}CH_2\text{-}OH$		$CH_3\text{-}CH_2\text{-}OH$		$[2\text{-}^2H_{0;2}, {}^{18}O_{1;0}]CH_3\text{-}CH_2\text{-}OH$
4.	$CH_3\text{-}CH^2H\text{-}OH$ $CH^2H_2\text{-}CH_2\text{-}OH$		$CH_3\text{-}CH_2\text{-}OH$		$[1\text{-}^2H_{1;0}, 2\text{-}^2H_{0;2}]CH_3\text{-}CH_2\text{-}OH$

1.28—An isotopically labeled compound is designated as *nonselectively labeled* when the position(s) and the number of the labeling nuclide(s) are both undefined.

In such cases the labeling is indicated by inserting the nuclide symbol, enclosed in square brackets, directly before the usual line formula with no locants or subscripts.

Example:

$[^{14}C]CH_3\text{-}CH_2\text{-}CH_2\text{-}CO_2H$

* Repetition of locants is not necessary as it may lead to ambiguity. Therefore, they have been omitted from this edition and a subscript added.

1.29—An isotopically labeled compound may be designated as *isotopically deficient* when the isotopic content of one or more elements has been depleted, i.e., when one or more nuclide(s) is(are) present in less than the natural ratio. Such an isotopically modified compound is denoted in the formula by adding the italicized syllable *def* immediately preceding, without a hyphen, the appropriate nuclide symbol.

Example:

$[def^{13}C]CHCl_3$

Note : According to one's viewpoint, one may also use $[^{12}C]CHCl_3$.

H-2. NAMES FOR ISOTOPICALLY MODIFIED COMPOUNDS

Rule H-2.1. Isotopically substituted compounds (cf. Rule H-1.23)

2.11—The name of an isotopically substituted compound is formed by inserting in *parentheses* (curves) the nuclide symbol(s), preceded by any necessary locant(s) (letters and/or numerals), before the name *or preferably* before the denomination of that part of the compound that is isotopically substituted. Immediately after the parentheses there is neither space nor hyphen, except that when the name, or a part of the name, includes a preceding locant, a hyphen is inserted. *

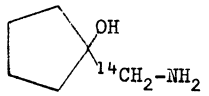
When polysubstitution is possible, the number of atoms substituted is always specified as a right subscript to the atomic symbol(s), even in case of monosubstitution.

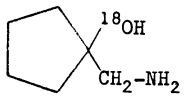
Examples:

1. $^{14}CH_4$ — (^{14}C)Methane

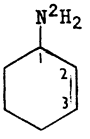
2. $CH_3{}^2H$ — ($^2H_1$)Methane

3. $C^2H_2Cl_2$ — Dichloro($^2H_2$)methane

4.  — 1-[Amino(^{14}C)methyl]cyclopentanol

5.  — 1-(Aminomethyl)cyclopentan(^{18}O)ol *or* 1-(Aminomethyl)(^{18}O)cyclopentanol

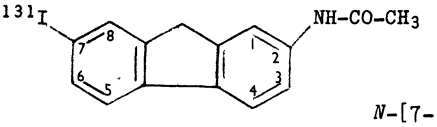
* In general, in organic nomenclature locants for suffixes, unsaturation, free valences, etc., cited ahead of the parent are considered as part of the name. In this report the practice of citing the isotopic descriptor ahead of such locants is followed; in biochemical usage the isotopic descriptor is often cited after such locants.

6. 

2-Cyclohexen-1-($^2H_2$)amine

or

(*N*,*N*-$^2H_2$)-2-Cyclohexen-1-amine

7. 

N-[7-(^{131}I)Iodofluoren-2-yl]acetamide

8. $^{14}CH_2$-$CO_2C_2H_5$
   $^{14}CH_2$-CO_2Na

Sodium ethyl (2,3-$^{14}C_2$)succinate

Rule H-2.2. Specifically labeled compounds (cf. Rule H-1.25)

2.21—The name of a specifically labeled compound is formed by inserting in *square brackets* the nuclide symbol(s), preceded by any necessary locant(s) (letters and/or numerals), before the name *or preferably* before the denomination of that part of the compound that is isotopically modified. Immediately after the brackets there is neither space nor hyphen, except that when the name, or a part of the name, requires a preceding locant, a hyphen is inserted. *

When polylabeling is possible, the number of atoms that have been labeled is always specified as a subscript to the atomic symbol(s), even in the case of monolabeling. This is necessary in order to distinguish between a specifically and a selectively or nonselectively labeled compound.

The name of a specifically labeled compound differs from the name of the corresponding isotopically substituted compound (see Rule H-2.11) only in the use of *square brackets* surrounding the nuclide descriptor rather than *parentheses* (curves).

Examples:

1. $[^{14}C]H_4$ — [^{14}C]Methane

2. $CH_3[^2H]$ — [$^2H_1$]Methane

3. $CH_3-CH_2-CH(CH_3)-CH=C[^2H_2]$ — 3-Methyl[1,1-$^2H_2$]-1-pentene †

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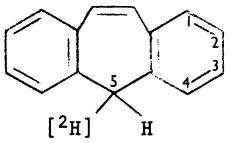
* See footnote, p. 518

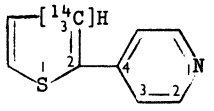
† Note that here the locant is part of the parent hydrocarbon name; see also footnote, p. 518

4.



[5-$^{2}H_{1}$]-5*H*-Dibenzo[*a*,*d*]cycloheptene *

5.



4-([3-^{14}C]-2-Thienyl)pyridine *

6. $C[^{2}H_{2}]Cl_{2}$

Dichloro[$^{2}H_{2}$]methane

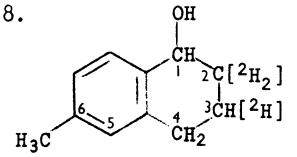
7. $CH_{3}-CH_{2}-O[^{2}H]$

Ethan[^{2}H]ol

or

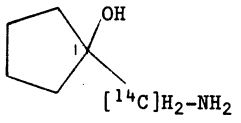
[*O*-^{2}H]Ethanol

8.



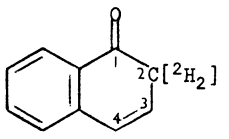
6-Methyl[2,2,3-$^{2}H_{3}$]-1,2,3,4-tetrahydro-1-naphthol †

9.



1-(Amino[^{14}C]methyl)cyclopentanol

10.



[2,2-$^{2}H_{2}$]-1(2*H*)-Naphthalenone

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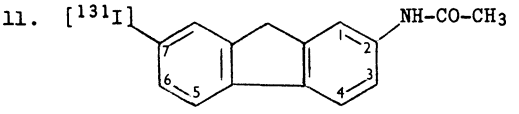
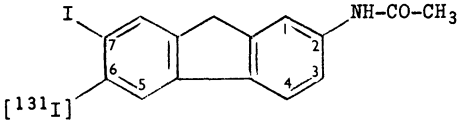
* Note that here the locant is part of the parent hydrocarbon or radical name; see also footnote, p. 518.

† In cases such as this, treatment of hydro prefixes as nondetachable is preferred; see Rule C-16.11, p. 108.

11. 

N-(7-[^{131}I]Iodofluoren-2-yl)acetamide

12. 

N-(6,7-[6-^{131}I]Diiodofluoren-2-yl)acetamide

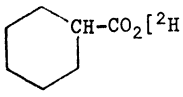
2.22—**In a name consisting of two or more words, the isotopic designator may be placed before** the appropriate word or part of the word that includes the labeled nuclide(s), unless unambiguous locants are available or are unnecessary.*

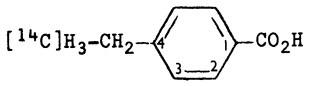
Examples:

1. $CH_2[^2H]\text{-}CO_2H$ — [2-$^2H_1$]Acetic acid

2. $CH_3\text{-}CO_2[^2H]$ — [*O*-^{2}H]Acetic acid
   or
   Acetic [^{2}H]acid

3. $CH_3\text{-}CH_2\text{-}CH_2\text{-}[^{14}C]O_2[^2H]$ — [1-^{14}C]Pentan[^{2}H]oic acid
   or
   [1-^{14}C, *O*-^{2}H]Pentanoic acid

4.  — Cyclohexane[^{2}H]carboxylic acid
   or
   [*O*-^{2}H]Cyclohexanecarboxylic acid

5.  — 4-([2-^{14}C]Ethyl)benzoic acid

6. $H\text{-}[^{14}C]O_2Na$ — Sodium [^{14}C]formate

7. $CH_3\text{-}CH_2\text{-}CO_2[^{14}C]H_2\text{-}CH_3$ — [1-^{14}C]Ethyl propionate

* The same rule applies to isotopically substituted compounds (see Rule H-2.11).

8. CH_3-[^{14}C]H_2-CO_2-CH_2-CH_3 Ethyl [2-^{14}C]propionate

9. $[C_6H_5N_2]^+[^{35}Cl]^-$ Benzenediazonium [^{35}Cl]chloride

2.23—In a trivial or semisystematic name consisting of one word, the isotopic designator may be placed before the full trivial name or inserted into the trivial name.

Examples:

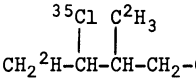
1. $(CH_3)_2CH-CH_2-[^{14}C]H(NH_2)-CO_2H$ [2-^{14}C]Leucine

2. $CH_3-[^{35}S]-CH_2-CH_2-CH(NH_2)-CO_2H$ [^{35}S]Methionine

3. $CH_3-CO-NH[^2H]$ [*N*-$^2H_1$]Acetamide
or
Acet[$^2H_1$]amide

Note: The alternative system based on the Boughton principles (see Introduction) denotes isotopic modification by citing the appropriate symbol and mass number (with subscripts and locants if necessary) *following* the portion of the name to which the symbol refers.

Example:



2-(Chloro-^{35}*Cl*)-3-(methyl-d_3)-pentane-*1-d*

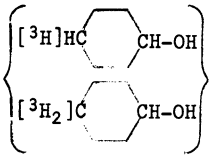
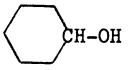
According to the rules recommended here, the name for this compound is : 2-(^{35}Cl)chloro-3-[($^2H_3$)methyl](1-$^2H_1$)pentane.

Rule H-2.3. Selectively labeled compounds (cf. Rules H-1.26 and H-1.27)

2.31—The name of a *selectively* labeled compound is formed in the same way as the name of a *specifically* labeled compound (see Rule H-2.21), except that the multiplying subscripts following the atomic symbols are generally omitted except as described by Rule H-2.32. Identical locants corresponding to the same element are not repeated.

The name of a selectively labeled compound differs from the name of the corresponding isotopically substituted compound in the use of *square brackets* surrounding the nuclide descriptor rather than parentheses (curves) and in the omission of repeated identical locants and multiplying subscripts.

Examples:

	Mixture of isotopically substituted compounds	when added to	is named
1.	$\{CH_3{}^2H,\ CH_2{}^2H_2,\ CH^2H_3,\ C^2H_4\}$	CH_4	[^{2}H]Methane *not* [$^2H_4$]Methane
2.	$\{CH_3-CH^2H-OH,\ CH_3-C^2H_2-OH\}$	CH_3-CH_2-OH	[1-^{2}H]Ethanol *not* [1,1-$^2H_2$]Ethanol
3.			[4-^{3}H]Cyclohexanol *not* [4,4-$^3H_2$]Cyclohexanol
4.	$\{^{14}CH_3-CH_2-CO_2-CH_2-CH_3,\ CH_3-CH_2CO_2-{}^{14}CH_2-CH_3\}$	$CH_3-CH_2-CO_2-CH_2-CH_3$	[1-^{14}C]Ethyl [3-^{14}C]propionate

2.32—In a selectively labeled compound formally arising from mixing several known isotopically substituted compounds with the analogous isotopically unmodified compound, the number or the possible number of labeling nuclide(s) for each position may be indicated by subscripts to the atomic symbol(s) as described in Rule H-1.27.

Examples:

	Mixture of isotopically substituted compounds	when added to	is named
1.	$\{CH_2{}^2H-CH_2-OH,\ CH^2H_2-CH_2-OH\}$	CH_3-CH_2-OH	[2-$^2H_{1;2}$]Ethanol
2.	$\{CH_3-CH_2-{}^{18}OH,\ CH^2H_2-CH_2-OH\}$	CH_3-CH_2-OH	[2-$^2H_{0;2}$,$^{18}O_{1;0}$]Ethanol

Rule H-2.4. Nonselectively labeled compounds (cf. Rule H-1.28)

2.41—The name of a nonselectively labeled compound is formed in the same way as the name of a selectively labeled compound (see Rule H-2.31) but contains neither locants nor subscripts in the nuclide descriptor.

Examples:

Chloro[^{3}H]benzene

[^{14}C]Glycerol

Rule H-2.5. Isotopically deficient compounds (cf. Rule H-1.29)

2.51—The name of an isotopically deficient compound may be formed by adding the italiziced syllable *def* immediately preceding, without a hyphen, the appropriate nuclide symbol, both enclosed in square brackets and cited before the name or that part of the name that is isotopically modified.

Example:

[*def*^{13}C]Chloroform

Rule H-2.6. General and uniform labeling

2.61—In the name of a selectively labeled compound in which *all* positions of the designated element are labeled, but not necessarily in the *same isotopic ratio*, the symbol "G" may be used in place of locants to indicate a "general" labeling.

Examples:

Isotopically substituted compounds	when added to	may be designated as
1. mixture of substituted compounds (selective labeling) $CH_3-CH_2-CH_2-{}^{14}CO_2H$ $CH_3-CH_2-{}^{14}CH_2-CO_2H$ $CH_3-{}^{14}CH_2-CH_2-CO_2H$ ${}^{14}CH_3-CH_2-CH_2-CO_2H$ $CH_3-{}^{14}CH_2-{}^{14}CH_2-CO_2H$ etc...	$CH_3-CH_2-CH_2-CO_2H$	[G-^{14}C]Butyric acid
2. D-Glucose in which all six positions are labeled with ^{14}C, but not necessarily uniformly, may be designated as D-[G-^{14}C]glucose.		

2.62—In the name of a selectively labeled compound in which *all* positions of the designated element are labeled in the *same isotopic ratio*, the symbol "U" may be used in place of locants to denote "uniform" labeling.

Examples:

Isotopically substituted compounds	when added to	may be designated as
1. mixture of substituted compounds (selective labeling) $\left\{\begin{array}{l}CH_3\text{-}CH_2\text{-}CH_2\text{-}{}^{14}CO_2H \\ CH_3\text{-}CH_2\text{-}{}^{14}CH_2\text{-}CO_2H \\ CH_3\text{-}{}^{14}CH_2\text{-}CH_2\text{-}CO_2H \\ {}^{14}CH_3\text{-}CH_2\text{-}CH_2\text{-}CO_2H \\ \text{in equal amounts}\end{array}\right\}$	$CH_3\text{-}CH_2\text{-}CH_2\text{-}CO_2H$	[U-^{14}C]Butyric acid
2. D-Glucose in which ^{14}C is equally distributed among the six positions		may be designated as D-[U-^{14}C]glucose.

Note: In the case of radioactive nuclides, "same isotopic ratio" means "same specific radioactivity".

2.63—In the name of a selectively labeled compound, the symbol "U" (see Rule H-2.62) followed by appropriate locants, may similarly be used to indicate labeling in the *same isotopic ratio at the specified positions*.

Example:

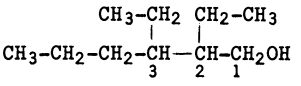
D-Glucose in which ^{14}C is equally distributed among positions 1, 3, and 5 may be designated as D-[U-= 1,3,5-^{14}C]glucose.

Rule H-2.7. Exceptional changes in the names of some unsymmetrically modified compounds

2.71—The name of an isotopically modified compound, substituted or labeled, may differ from the name of the unmodified analog when its structure includes identical units that are not identically modified in equivalent positions. Where there is ambiguity, such different groups must be expressed separately.

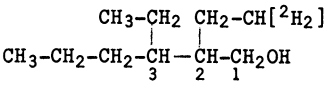
Example:

Unmodified compound:



2,3-Diethyl-1-hexanol

Modified compound:



2-([2,2-$^{2}H_{2}$]Ethyl)-3-ethyl-1-hexanol

Rule H-2.8. Order of nuclide symbols

2.81—When isotopes of different elements are present as nuclides in an isotopically modified compound, their symbols are arranged in alphabetical order if they are inserted at the same place in the name.

Examples:

1. Mixed substituted compound

   $CH_3{}^{18}O{}^{2}H$ — Methan(^{2}H,^{18}O)ol

   or

   (*O*-^{2}H,^{18}O)Methanol

2. Mixed specifically labeled compounds

   a. $CH_3[^{18}O][^{2}H]$ — Methan[^{2}H,^{18}O]ol

   or

   [*O*-^{2}H,^{18}O]Methanol

   b. $H_2[^{15}N]$-$[^{14}C]$O-NH[^{2}H] — [^{14}C,*N*'-$^{2}H_1$,*N*-^{15}N]Urea *

3. Mixed selectively labeled compound

   D-Glucose labeled uniformly with ^{14}C and generally with ^{2}H — D-[U-^{14}C,G-^{2}H]Glucose

2.82—When several isotopes of the same element are present as nuclides in an isotopically modified compound, their symbols are arranged in the order of increasing atomic mass number if they are inserted at the same place in the name.

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* For numbering priority between *N* and *N*', see Rule H-3.21.

Examples:

1. Mixed substituted compound

   $CH_2{}^2H\text{-}CH^3H\text{-}OH$ $(2\text{-}^2H_1,1\text{-}^3H_1)$Ethanol

2. Mixed specifically labeled compounds

   a. $CH_2[^2H]\text{-}OH$, $CH_2[^3H]\text{-}OH$ $[^2H_1,^3H_1]$Methanol

   b. $CH_3\text{-}O[^2H]$, $CH_3\text{-}O[^3H]$ Methan$[^2H,^3H]$ol

   or

   $[O\text{-}^2H,O\text{-}^3H]$Methanol

   c. $CH_2[^2H]\text{-}CH_2\text{-}CH[^3H]\text{-}CO_2H$ $[4\text{-}^2H_1,2\text{-}^3H_1]$Butyric acid

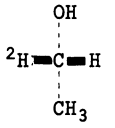
Rule H-2.9. Stereoisomeric isotopically modified compounds

2.91—Two types of stereoisomeric isotopically modified compounds are possible: (a) those in which the stereoisomerism results from isotopic modification, and (b) those whose analogous unmodified compounds are stereoisomers.

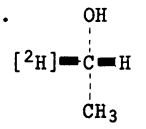
The nomenclature of stereoisomers of isotopically modified compounds follows the general methods of stereochemical nomenclature as described in Section E.

Stereochemical affixes are cited at the specified place in the name according to the stereochemical rules. When they must be inserted into the name at the same place as isotopic descriptors, the stereochemical affixes are cited first.

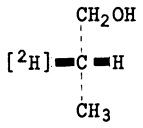
Examples in which stereoisomerism results from isotopic modification:

1. 

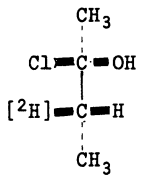
   $(S)\text{-}(1\text{-}^2H_1)$Ethanol

2. 

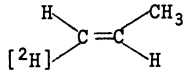
   $(S)\text{-}[1\text{-}^2H_1]$Ethanol

3. 

(*S*)-[2-$^2H_1$]-1-Propanol

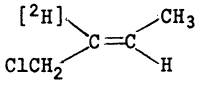
4. 

(2*R*,3*S*)-2-Chloro[3-$^2H_1$]-2-butanol

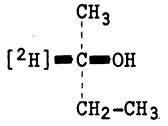
5. 

(*E*)-[1-$^2H_1$]Propene

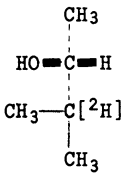
Examples of isotopically modified stereoisomers:

6. 

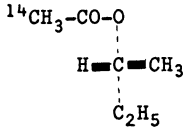
(*E*)-1-Chloro[2-^{2}H]-2-butene

7. 

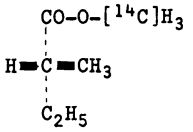
(*S*)-[2-^{2}H]-2-Butanol

8. 

(*R*)-3-Methyl[3-^{2}H]-2-butanol

9. 

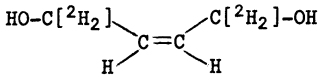
(*R*)-*sec*-Butyl (2-^{14}C)acetate

10. 

[^{14}C]Methyl (*R*)-2-methylbutyrate

or

(*R*)-([^{14}C]Methyl 2-methylbutyrate)

11. 

(*Z*)-[1,1,4,4-$^{2}H_4$]-2-Butene-1,4-diol

2.92 **Stereochemical affixes** (for example D and L) added according to the rules of special classes, such as carbohydrates, amino acids, steroids, etc., usually refer to **the parent substance** (or unmodified compound) according to the particular class of compounds. However, isotopic descriptors follow the stereochemical descriptors in these classes, according to biochemical usage.*

Examples:

1. L-[3,4-^{13}C,^{35}S]Methionine

2. L-[3-^{14}C,2,3-$^{2}H_2$,^{15}N]Serine

3. 5α-[17-^{2}H]Pregnane

4. (24*R*)-5α-[24-$^{2}H_1$]Cholestane

5. 2-([^{18}F]Fluoro)-2-deoxy-D-glucose

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* See footnote, p.518

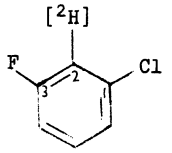
H-3. NUMBERING OF ISOTOPICALLY MODIFIED COMPOUNDS

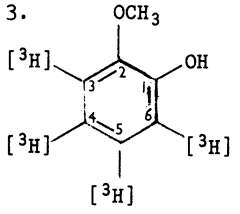
Rule H-3.1. Numbering in relation to the unmodified compound

3.11—Numbering of an isotopically modified compound is *not* changed from that of an isotopically unmodified compound. Among the structural features of a compound to be considered successively for numbering as given by the Rule C-15.11, p. 105 and Section E , the presence of nuclides is considered last with the exception of chirality arising from isotopic modification (see Rule H-3.22, example 7).

Examples:

1. $CF_3-CH_2[^2H]$ — 1,1,1-Trifluoro[$^2H_1$]ethane

2.  — 1-Chloro-3-fluoro[2-^{2}H]benzene

3.  — 2-Methoxy[3,4,5,6-$^3H_4$]phenol

Note: One should be aware that, when isotopically modified compounds are named by the system based on an extension of the Boughton principles (see Introduction, p. 513), lowest locants are assigned to isotopic positions included in the parent structure, which includes unsaturation and principal groups, if any, before other considerations. This sometimes results in the assignment of higher locants for substituents expressed by prefixes, which may give a numbering that differs from the one assigned according to Rule H-3.1.

Example:

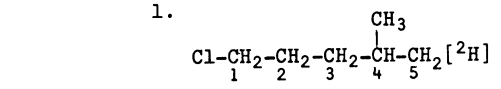
$F_3C-CH_2{}^2H$ — 2,2,2-Trifluoroethane-*1-d*

Note that here the presence of deuterium (*d*) causes the carbon atom to which it is attached to be assigned the locant 1. For more details and examples see ref. 4.

Rule H-3.2. Priority between isotopically modified and unmodified atoms or groups

3.21—When there is a choice between equivalent posssibilities for the principal chain or senior cyclic system in an isotopically unmodified compound, the principal chain or senior cyclic system of the analogous isotopically modified compound is chosen so as to include the maximum number of modified atoms or groups. If a choice still remains, precedence is given to the principal chain or senior ring that contains a nuclide of higher atomic number. In case of different nuclides of the same element, precedence is given to a nuclide of higher mass number.

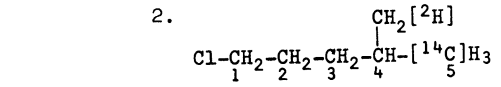
Examples:

1. 

1-Chloro-4-methyl[5-$^{2}H_{1}$]pentane

not

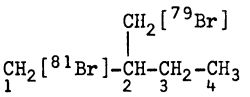
1-Chloro-4-([$^{2}H_{1}$]methyl)pentane

2. 

1-Chloro-4-([$^{2}H_{1}$]methyl)[5-^{14}C]pentane

not

1-Chloro-4-([^{14}C]methyl)[5-$^{2}H_{1}$]pentane

3. 

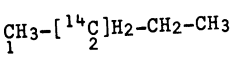
1-([^{81}Br]Bromo)-2-([^{79}Br]bromomethyl)butane

not

1-([^{79}Br]Bromo)-2-([^{81}Br]bromomethyl)butane

3.22—When there is a choice between equivalent numberings in an isotopically unmodified compound, the starting point and direction of numbering of the analogous isotopically modified compound are chosen so as to give lowest locants to the *modified* atoms or groups considered together in one series in ascending numerical order (see Rule C-15.11 p. 105). If a choice still remains, precedence for the lowest locants is given to a nuclide of higher atomic number. In the case of different nuclides of the same element, precedence is given to the nuclide of higher mass number.

Examples:

1. 

[2-^{14}C]Butane

not

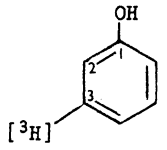
[3-^{14}C]Butane

2. $\overset{1}{CH_3}-\overset{2}{C}[^2H_2]-[^{14}\overset{3}{C}]H_2-\overset{4}{CH_3}$

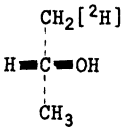
[3-^{14}C,2,2-$^2H_2$]Butane
not
[2-^{14}C,3,3-$^2H_2$]Butane

3. $\overset{1}{CH_3}-[^{14}\overset{2}{C}]H_2-\overset{3}{CH}[^2H]-\overset{4}{CH_3}$

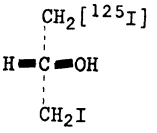
[2-^{14}C,3-$^2H_1$]Butane
not
[3-^{14}C,2-$^2H_1$]Butane

4. 

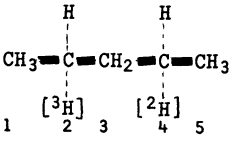
[3-^{3}H]Phenol

5. 

(*R*)-[1-$^2H_1$]-2-Propanol

6. 

(*S*)-1,3-[1-^{125}I]Diiodo-2-propanol

7. 

(2*S*,4*R*)-[4-$^2H_1$,2-$^3H_1$]Pentane
not
(2*R*,4*S*)-[2-$^2H_1$,4-$^3H_1$]Pentane

Note: In the last example above, the numbering follows Rule H-3.22 rather than the stereochemical preferences as described in Rules of Section E , which give preference to *R* groups over *S* groups for lowest locants.

H-4. LOCANTS FOR NUCLIDES IN ISOTOPICALLY MODIFIED COMPOUNDS

Rule H-4.1. Omission or introduction of locants

4.11—When there is no ambiguity, locants may be omitted from the isotopic designator in the name of an isotopically modified compound.

Examples:

1. $C[^2H_3]$-CN — [$^2H_3$]Acetonitrile

2. CH_3-NH[^2H] — Methyl[$^2H_1$]amine

3. CH_3-CH_2-O[^2H] — Ethan[^2H]ol

4. [^2H]O-CH_2-CH_2-O[^2H] — 1,2-Ethane[$^2H_2$]diol

5. $CH_2[^2H]$-O-$C[^2H_2]$-S-CH_2-OOH — [([$^2H_1$]Methoxy[$^2H_2$]methyl)thio]methyl hydroperoxide

4.12—When ambiguity may occur, specific positions of nuclides should be indicated in the isotopic designator by appropriate locants, letters and/or numerals, preceding the nuclide symbol(s).

Examples (see also Rules H-2.11, H-2.21, H-2.31):

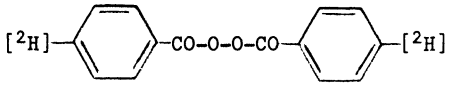
1. $C[^2H_3]$-NH_2 — [1,1,1-$^2H_3$]Methylamine

2. CH_3-CH[^2H]-OH — [1-$^2H_1$]Ethanol

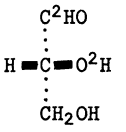
3. HO-CH[^2H]-CH[^2H]-OH — [1,2-$^2H_2$]-1,2-Ethanediol

4. $C[^2H_3]$-C(=O)-$C[^2H_2]$-CH_2-CH_3 — [1,1,1,3,3-$^2H_5$]-2-Pentanone

5. CH_3-CH(SH)-CH[^2H]-CH_3 — [3-$^2H_1$]-2-Butanethiol

6. 

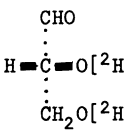
Di([4-^2H]benzoyl) peroxide

7. 

(*R*)-(*O*^{2},1-$^2H_2$)Glyceraldehyde

or

(*R*)-(*O*-^{2}H)Glycer(^{2}H)aldehyde

8. 

(*R*)-[*O*^{2},*O*^{3}-$^2H_2$]Glyceraldehyde

9. [^{2}H]S-CH_2-CH(N[$^2H_2$])-CO_2[^{2}H]

DL-[*N*,*N*,*O*,*S*-$^2H_4$]Cysteine

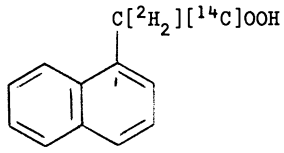
Rule H-4.2. Location of nuclides on positions of compounds that are normally not assigned locants (letters or numerals)

4.21—When a nuclide occupies a position that is not numbered, an italicized prefix or Greek letter may be used to denote its position.

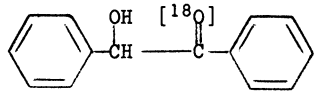
Examples:

1. [$^2H_3$][^{14}C]-S-CH_2-CH_2-CH(NH_2)-COOH

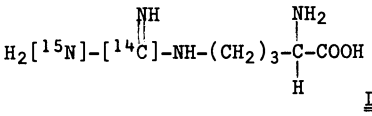
DL-[*methyl*-(^{14}C,$^2H_3$)]Methionine

2. 

1-Naphthalene[*carboxy*-^{14}C,α,α-$^2H_2$]acetic acid

3. 

[*carbonyl*-^{18}O]Benzoin

4. 

L-[*guanidino*-^{14}C,*N*^{3}-^{15}N]Arginine

4.22—When a nuclide occupies a position that is not numbered or when its position cannot be easily defined according to Rules H-4.12 and H-4.21, the nuclide symbol may be included in the entire symbol of the group through which it is linked to the main part of the structure.

Examples:

1. $CH_3-CH_2-S-[^{34}S]-S-(CH_2)_2-CO_2H$

3-(Ethyl[S-^{34}S-S]trithio)propionic acid

or

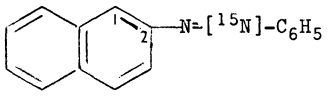
3-(Ethyl[2-^{34}S]trisulfanyl)propionic acid *

2. $CH_3-CH_2-[^{34}S]-S-S-(CH_2)_2-CO_2H$

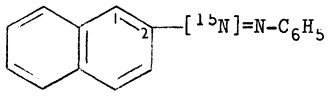
3-(Ethyl[^{34}S-S-S]trithio)propionic acid

or

3-(Ethyl[3-^{34}S]trisulfanyl)propionic acid *

3. 

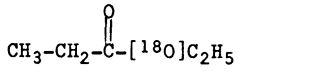
Naphthalene-2-[N=^{15}N]azobenzene

4. 

Naphthalene-2-[^{15}N=N]azobenzene

4.23—Italicized nuclide symbols and/or capital italic letters may be used as locants to distinguish between different nuclides of the same element.

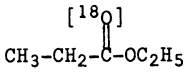
Examples:

1. 

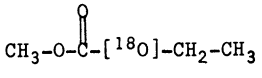
^{18}O-Ethyl [$^{18}O_1$]propionate

* See Rule C-515.2, p. 216.

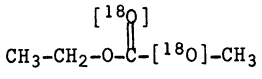
Examples (cont.):

2. 

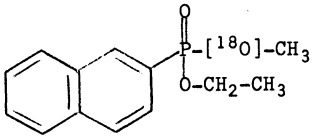
O-Ethyl [$^{18}O_1$]propionate

3. 

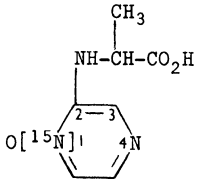
^{18}*O*-Ethyl *O*-methyl [$^{18}O_1$]carbonate

4. 

O-Ethyl ^{18}*O*-methyl [$^{18}O_2$]carbonate

5. 

O-Ethyl ^{18}*O*-methyl 2-naphthyl[$^{18}O_1$]phosphonate

6. 

N-([1-^{15}N]-2-Pyrazinyl)alanine ^{15}*N*-oxide

References

1. I.U.P.A.C. Manual of Symbols and Terminology for Physicochemical Quantities and Units, 1973 Edition, Butterworths, London, 1975, Rules 7.1 and 7.2, p. 24.

2. I.U.P.A.C. Commission on Atomic Weights, *Pure and Applied Chemistry*, 37, 591-603 (1974).

3. (a) W. A. Boughton, Naming Hydrogen Isotopes, *Science*, 79, 159-60 (1934); (b) E. J. Crane, Nomenclature of the Hydrogen Isotopes and Their Compounds, *Science*, 80, 86-9 (1934); (c) American Chemical Society, Report of Committee on Nomenclature, Spelling, and Pronunciation, Nomenclature of the Hydrogen Isotopes and Their Compounds, *Ind. Eng. Chem.* (News Ed.), 13, 200-1 (1935).

4. "The Naming and Indexing of Chemical Substances for Chemical Abstracts During the Ninth Collective Period (1972-1976)", ¶220, p. 111I, a reprint of Section IV of the Introduction to the Chemical Abstracts Volume 76 Index Guide.

5. I.U.P.A.C. Nomenclature of Inorganic Chemistry, 2nd Edition (1970), Butterworths, London, 1971: (a) Rule 1.31, p. 11; (b) Rule 1.1, p. 10.

APPENDIX

Comparative Examples of Formulae and Names for Isotopically Modified Compounds

Type of Compound	Formula	Name
Unmodified	CH_3-CH_2-OH	Ethanol
Isotopically substituted	C^2H_3-CH_2-O^2H	(2,2,2-$^2H_3$)Ethan(^{2}H)ol *or* (*O*,2,2,2-$^2H_4$)Ethanol
Specifically labeled	$C[^2H_3]$-CH_2-$O[^2H]$	[2,2,2-$^2H_3$]Ethan[^{2}H]ol *or* [*O*,2,2,2-$^2H_4$]Ethanol
Selectively labeled	a. [*O*,2-^{2}H]CH_3-CH_2-OH b. [2-$^2H_{2;2}$, $^{18}O_{0;1}$]CH_3-CH_2-OH	a. [*O*,2-^{2}H]Ethanol b. [2-$^2H_{2;2}$, $^{18}O_{0;1}$]Ethanol
Nonselectively labeled	[^{2}H]CH_3-CH_2-OH	[^{2}H]Ethanol
Isotopically deficient	[*def*^{13}C]CH_3-CH_2-OH	[*def*^{13}C]Ethanol